INTERNATIONAL STANDARD 2131

INTERNATIONAL ORGANIZATION FOR STANDARDIZATION • МЕЖДУНАРОДНАЯ ОРГАНИЗАЦИЯ ПО СТАНДАРТИЗАЦИИ • ORGANISATION INTERNATIONALE DE NORMALISATION

Surface active agents — Simplified classification

First edition — 1972-11-01

UDC 661.185 : 168.2

Ref. No. ISO 2131-1972 (E)

Descriptors : surfactants, classifying

Price based on 5 pages

FOREWORD

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Draft International Standards adopted by the Technical Committees are circulated to the Member Bodies for approval before their acceptance as International Standards by the ISO Council.

International Standard ISO 2131 was drawn up by Technical Committee ISO/TC 91, *Surface active agents.*

It was approved in June 1971 by the Member Bodies of the following countries :

Australia	Japan	Spain
Austria	Korea, Rep. of	Switzerland
Belgium	New Zealand	Thailand
Egypt, Arab Rep. of	Poland	Turkey
France	Portugal	United Kingdom
Germany	Romania	U.S.A.
Israel	South Africa, Rep. of	U.S.S.R.

No Member Body expressed disapproval of the document.

Printed in Switzerland

Surface active agents – Simplified classification

1 SCOPE AND FIELD OF APPLICATION

This International Standard establishes a simplified classification of surface active agents, in conformity, regarding the arrangement of radicals, with the scientific classification (ISO/R 896).

2 PRINCIPLE

The simplified classification of surface active agents enables their characteristics to be expressed by an abbreviated lettering and numbering system, consisting of a letter and four figures (five in the case of compounds comprising several hydrophilic groups), for the main structural elements of the molecule, using

1) the letter to designate the ionic character;

2) the 1st figure to designate the hydrophilic group;

3) the 2nd figure to designate the hydrophobic group;

4) the 3rd figure to designate an intermediate functional group;

5) the 4th figure to designate a supplementary property of the hydrophilic group;

6) the 5th figure (in parentheses between the 1st and 2nd) to designate the second hydrophilic group of compounds comprising several hydrophilic groups of different ionic characters.

The operation is carried out by determining, from the classification Table given in the Annex arising from the general scientific classification, the figures which correspond to the groups present in the molecule, by the application of the rules defined in section 3.

3 RULES OF CLASSIFICATION

3.1 Choice of the hydrophilic group

Rule 1

The hydrophilic group is the point of departure for the classification. Its ionic character shall be designated by one of the following letters :

A for anionic hydrophilic groups;

C for cationic hydrophilic groups;

N for non-ionic hydrophilic groups;

Z for true ampholytic compounds.

Rule 2

In the presence of several hydrophilic groups with identical ionic characters, select as the principal hydrophilic group that which is designated first in the following numbering order, with reference to the divisions in the Table in the Annex :

for groups which are

– anionic : 2 – 3 – 4 – 5 – 6 – 7 – 8 – 9 – 1

– cationic : 5 – 6 – 7 – 8 – 9 – 1 – 2 – 3 – 4

– non-ionic : 3 – 4 – 5 – 6 – 1 – 2 – 7 – 8 – 9

Rule 3

In the presence of several hydrophilic groups with different ionic characters, two alternatives must be considered :

a) in the presence of anionic and cationic groups (ampholytic compounds), use the letter Z. Designate the cationic group first and the anionic group second, in parentheses, applying Rule 2 if necessary;

b) in the presence of an ionic group and a non-ionic group, use as the letter that which characterises the ionic group. Designate this first and the non-ionic group second, in parentheses, applying Rule 2 if necessary.

3.2 Choice of the hydrophobic group

Rule 4

The determinant hydrophobic group is the most important radical for the hydrophobic behaviour; in general, it is usually the longest hydrocarbon chain (including rings), as far removed as possible from the principal hydrophilic group.

Rule 5

An aliphatic hydrocarbon chain shall be regarded as sufficiently long, in the terms of Rule 4, if it consists of at least 8 carbon atoms.

Rule 6

If the surface active agent does not contain a hydrocarbon chain with at least 8 carbon atoms, take a cyclic residue as the determinant hydrophobic group.

3.3 Choice of the intermediate functional group

Rule 7

Choose as the intermediate functional group the one which is nearest to the principal hydrophilic group.

NOTE – The most important surface active agents correspond to the formula

$$R - X - R' - F$$

in which the letters F, R′, X in the Table given in the Annex have the following meaning :

R indicates the principal hydrophobic group;

X indicates an intermediate function;

R′ indicates a short hydrocarbon chain;

F indicates the principal hydrophilic group.

The letters F, R′, X in the Table given in the Annex have the same meaning; on the other hand the letter r, used also in the table, indicates a hydrogen or alkyl residue.

3.4 Choice of the supplementary property of the hydrophilic group

Rule 8

The supplementary property of the hydrophilic group shall be that of the principal hydrophilic group; it shall be selected in accordance with the numbering order in the Table.

3.5 Note

Should it appear necessary to record the classification on punched cards or a computer, any parentheses there may be should disappear. In the case of compounds having two or more hydrophilic groups with identical ionic characters, insert 0 between the first and second figures obtained. In the case of compounds having several groups of different ionic characters, merely omit the parentheses.

Example A 1031 (see Appendix, section Z.1) becomes A 10031 and example Z 2(1)002 (see Appendix, section Z.4) becomes Z 21002.

ANNEX

TABLE — **Simplified classification of surface active agents**

Hydrophilic group			Determinant hydrophobic group	Intermediate functional group	Supplementary properties of the hydrophilic group		
anionic	cationic	non-ionic			anionic	cationic	non-ionic
			0 Non-branched aliphatic residue	0 Absence of	0 Absence of	0 Absence of	0 Absence of
1 $-COOH$	1 Primary amine	1 Aliphatic hydroxyl group	1 Branched aliphatic residue	1 $-COO-R'-F$	1 Alkaline metal salts Li, Na, K etc. (Group Ia)	1 1 or 2 hydrophobic residues. Inorganic anion	1 Characterising hydroxyl function
2 $-OSO_3H$	2 Secondary amine	2 Alicyclic or aromatic hydroxyl group	2 Alicyclic residue terpenes	2 $-OOC-R'-F$	2 Alkaline earth metal salts Mg, Ca, Sr, Ba etc. (Group IIa)	2 1 or 2 hydrophobic residues. Organic anion	2 Characterising ester function
3 $-SO_3H$	3 Tertiary amine	3 Non-branched poly-ether on inter-mediate chain	3 Non-condensed benzene residue	3 $-CON(r)-R'-F$ $-N(r)CO-R'-F$ 1 and 2 intermediate functions	3 Salts of metal Cu, Ag, Zn, Cd, Hg (Groups Ib and IIb)	3 1 or 2 hydrophibic residues. Benzyl radical and similar. Inorganic anion	3 Characterising ester function
4 $-S-SO_3H$	4 Amino oxide	4 Branched polyether on intermediate chain	4 Aromatic residue with condensed rings	4 $-SO_2N(r)-R'-F$ $-N(r)SO_2-R'-F$	4 Transition metal salts Cr, Mn, Fe, Co, Ni (Groups VIa, VIIa, VIII)	4 1 or 2 hydrophobic residues. Benzyl radical and similar. Organic anion	4 Characterising amide function
5 $-SO_2H$ Other sulphur functions, including $-SO_2NH(r)$	5 Quaternary ammonium	5 Derivatives of sorbitan, mannitan, carbohydrates and similar	5 Heterocyclic residue with 1 non-carbon atom on the ring	5 $-O-R'-(O-R')_nF$ 1, 2 and 3 inter-mediate functions	5 Salts of metals Al, In, Sn, Pb, Bi (Groups IIIb to Vb)	5 Three hydrophobic residues. Inorganic anion	5 Characterising sulphamide function $-SO_2N(r)_2$
6 Orthophosphoric acid esters	6 Pyridinium imidazolinium and similar	6 Derivatives of sorbitan, mannitan, oxy alkyl carbo-hydrates	6 Heterocyclic residue with 2 or more non-carbon atoms on the ring	6 $-S-R'-F$ $-SO-R'-F$ $-SO_2-R'-F$	6 Lanthanum and acti-nium group metal salts La, Ce, Th, U etc.	6 Three hydrophobic residues. Organic anion	6
7 Phosphonic acids	7 Sulphonium	7 Carbonyl group	7 Polymer residue	7 $-N(r)-R'-F$	7 Ammonium salts	7 Metallic complexes	7
8 Per acids	8 Phosphonium	8 Urea, ureides, polypeptides	8 Residue containing other elements in chain	8 Others $-X-R'-F$	8 Organic base salts	8 Betaines	8 Organo-metallic derivatives
9 Other anionic functions	9 Other cationic functions	9 Other non-ionic functions	9 Other hydrophobic residues	9	9 Salts of complex metals. Organo-metallic bases	9 Other specialized characteristics	9 Other character-ising functions

APPENDIX

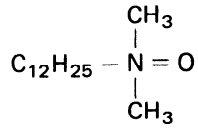
EXAMPLES OF APPLICATION OF THE SIMPLIFIED CLASSIFICATION

Z.1 ANIONIC SURFACE ACTIVE AGENTS

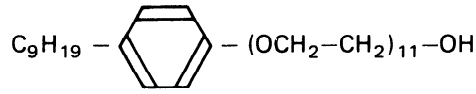
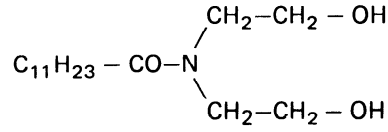
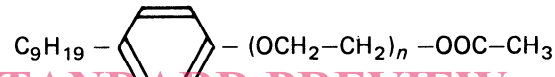
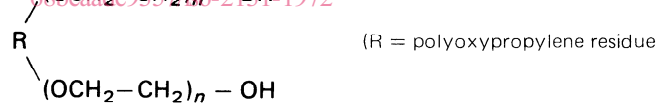
Sodium stearate	$C_{17}H_{35}COONa$	A 1001
Sodium lauroyl sarcosinate	$C_{11}H_{23}-CO-N(CH_3)-CH_2-COONa$	A 1031
Sodium laurylsulphate	$C_{12}H_{25}-OSO_3Na$	A 2001
Sodium lauryl ethoxy-ether sulphate	$C_{12}H_{25}-OCH_2-CH_2-OCH_2-CH_2-OSO_3Na$	A 2051
Sodium salt of the sulphuric ester of lauroyl ethanolamide	$C_{11}H_{23}-CO-NH-CH_2-CH_2-OSO_3Na$	A 2031
Sodium alkylsulphonate	$C_{11}H_{23}-CH(SO_3Na)-C_2H_5$	A 3001
Sodium oleyl-oxyethane sulphonate	$C_{17}H_{33}-COO-CH_2-CH_2-SO_3Na$	A 3011
Sodium salt of oleyl-methyltauride	$C_{17}H_{33}-CO-N(CH_3)-CH_2-CH_2-SO_3Na$	A 3031
Sodium alkylaryl-sulphonate	$C_{12}H_{25}-C_6H_4-SO_3Na$	A 3301
Sodium mono-alkylphosphate	$C_{12}H_{25}-O-P(=O)(ONa)_2$	A 6001
Sodium dioctylsulphosuccinate	$C_8H_{17}-OOC-CH_2-CH(COO-C_8H_{17})-SO_3Na$	A 3021

Z.2 CATIONIC SURFACE ACTIVE AGENTS

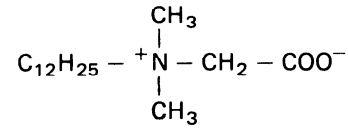
Stearyl-dimethyl-benzyl-ammonium chloride	$[C_{18}H_{37}-N(CH_3)_2-CH_2-C_6H_5]^+ Cl^-$	C 5003
Imidazoline acetate alkyl substituted	$C_{17}H_{33}-C(=N-CH_2)-N(-CH_2-CH_2OH)-CH_2$, $HOOC-CH_3$	C 6002
Stearoyl-amidoethyl-trimethylammonium methosulphate	$[C_{17}H_{35}-CO-NH-CH_2-CH_2-N(CH_3)_3]^+ OSO_3CH_3^-$	C 5031

Dimethyl-laurylamine oxide		C 4000

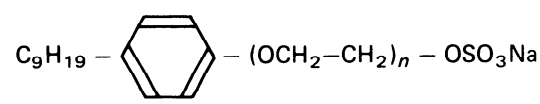
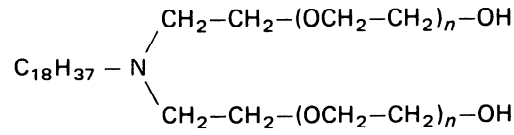
Z.3 NON-IONIC SURFACE ACTIVE AGENTS

Sorbitol fatty acid esters	$C_{11}H_{23}-CO-OCH_2(CHOH)_4CH_2OH$	N 5010
Polyethoxylated stearyl alcohol	$C_{18}H_{37}-(OCH_2-CH_2)_{20}-OH$	N 3001
Polyethoxylated stearic acid	$C_{17}H_{35}-CO-OCH_2-CH_2-(OCH_2-CH_2)_5-OH$	N 3011
Polyethoxylated nonylphenol		N 3301
Lauroyl-diethanolamide		N 1031
Polyethoxylated nonylphenol acetate		N 3302
Methoxy-polyethylene-oxy-nonylphenol		N 3303
Pluronics	 (R = polyoxypropylene residue)	N 3701

Z.4 AMPHOLYTE SURFACE ACTIVE AGENTS

Sodium *n*-laurylamino-propionate	$C_{12}H_{25}-NH-CH_2-CH_2-COONa$	Z 2(1)002
Dimethyl-dodecyl-betaine acetate		Z 5(1)008

Z.5 SURFACE ACTIVE AGENTS WITH IONIC AND NON-IONIC HYDROPHILIC GROUPS

Sodium salt of polyethoxylated nonylphenol sulphate		A 2(3)301
Polyethoxylated stearylamine		C 3(3)000

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